



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 09:57 PM UTC

PDB ID : 2VSS / pdb_00002vss
Title : Wild-type Hydroxycinnamoyl-CoA hydratase lyase in complex with acetyl-CoA and vanillin
Authors : Bennett, J.P.; Bertin, L.M.; Brzozowski, A.M.; Walton, N.J.; Grogan, G.
Deposited on : 2008-04-29
Resolution : 2.22 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

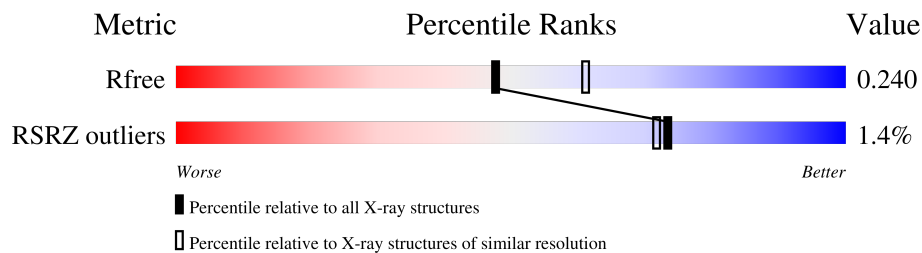
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11928 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called P-HYDROXYCINNAMOYL COA HYDRATASE/LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	239	1847	1170	320	344	13	0	1	1
1	B	248	1943	1233	336	362	12	0	0	1
1	C	236	1821	1151	319	339	12	0	1	1
1	D	246	1957	1242	342	361	12	0	2	0

- Molecule 2 is a protein called P-HYDROXYCINNAMOYL COA HYDRATASE/LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	241	1887	1199	325	350	13	0	1	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	146	TYR	TRP	conflict	UNP O69762

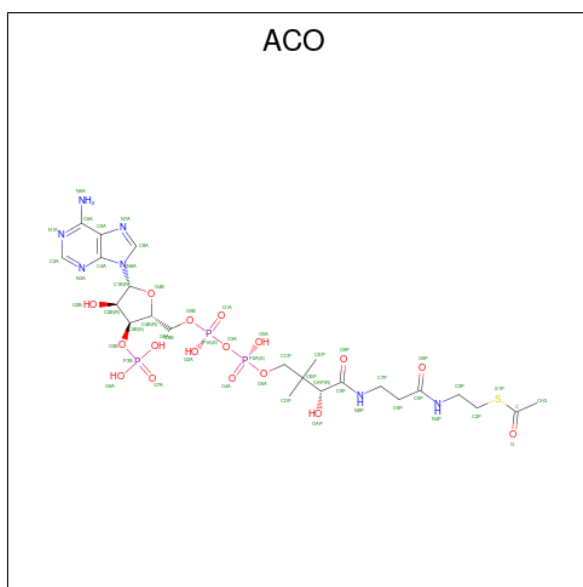
- Molecule 3 is a protein called P-HYDROXYCINNAMOYL COA HYDRATASE/LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	247	1942	1234	337	359	12	0	1	1

There is a discrepancy between the modelled and reference sequences:

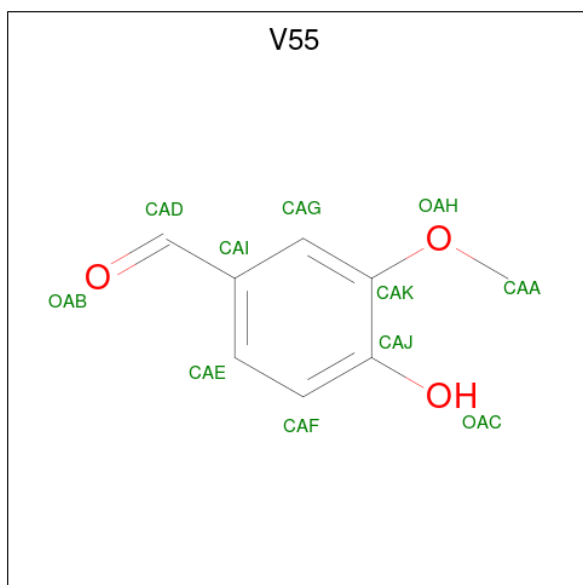
Chain	Residue	Modelled	Actual	Comment	Reference
F	29	ARG	LYS	conflict	UNP O69762

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
			Total	C	N	O	P			S	
4	B	1	Total	51	23	7	17	3	1	0	0
4	D	1	Total	51	23	7	17	3	1	0	0
4	E	1	Total	51	23	7	17	3	1	0	0
4	F	1	Total	51	23	7	17	3	1	0	0

- Molecule 5 is 4-hydroxy-3-methoxybenzaldehyde (CCD ID: V55) (formula: $C_8H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			11	8	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	35	Total	O	0	0
			35	35		
6	B	60	Total	O	0	0
			60	60		
6	C	38	Total	O	0	0
			38	38		
6	D	60	Total	O	0	0
			60	60		
6	E	61	Total	O	0	0
			61	61		
6	F	62	Total	O	0	0
			62	62		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.22Å 130.59Å 144.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.13 – 2.22 96.94 – 2.22	Depositor EDS
% Data completeness (in resolution range)	91.5 (97.13-2.22) 91.6 (96.94-2.22)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.22Å)	Xtrriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.183 , 0.242 0.182 , 0.240	Depositor DCC
R_{free} test set	3933 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.559	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11928	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACO	F	1249	-	51,53,53	1.77	10 (19%)	73,79,79	2.34	22 (30%)
4	ACO	B	1251	-	51,53,53	1.39	9 (17%)	73,79,79	1.83	20 (27%)
4	ACO	D	1249	-	51,53,53	1.67	7 (13%)	73,79,79	1.81	18 (24%)
4	ACO	E	1250	-	51,53,53	1.66	9 (17%)	73,79,79	2.05	20 (27%)
5	V55	D	1250	-	11,11,11	1.11	0	14,14,14	1.72	5 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACO	F	1249	-	-	13/51/67/67	0/3/3/3
4	ACO	B	1251	-	-	3/51/67/67	0/3/3/3
4	ACO	D	1249	-	-	1/51/67/67	0/3/3/3
4	ACO	E	1250	-	-	8/51/67/67	0/3/3/3
5	V55	D	1250	-	-	0/4/4/4	0/1/1/1

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1249	ACO	C-S1P	5.72	2.06	1.75
4	F	1249	ACO	P1A-O3A	5.28	1.65	1.59
4	F	1249	ACO	C-S1P	4.98	2.02	1.75
4	E	1250	ACO	P3B-O3B	4.78	1.67	1.59
4	E	1250	ACO	P1A-O1A	4.56	1.66	1.50

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1249	ACO	C7P-N8P-C9P	-10.31	104.02	122.55
4	E	1250	ACO	C3P-N4P-C5P	6.07	134.13	122.82
4	F	1249	ACO	N3A-C2A-N1A	-5.60	120.10	128.58
4	B	1251	ACO	N3A-C2A-N1A	-5.57	120.14	128.58
4	D	1249	ACO	C5A-C4A-N3A	-5.25	119.48	126.72

There are no chirality outliers.

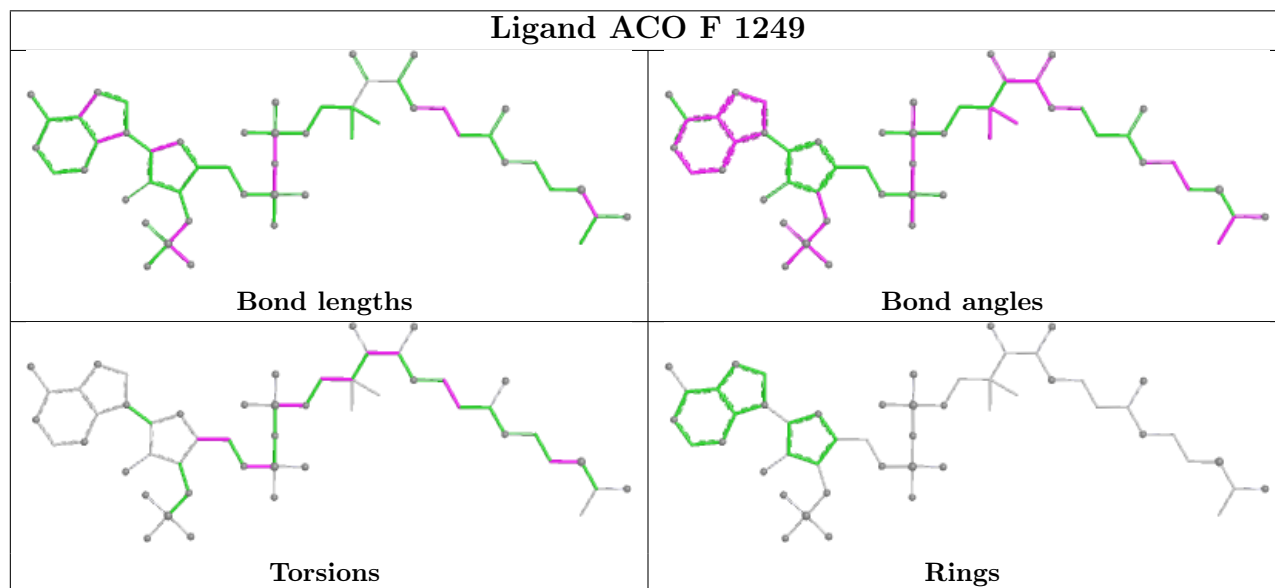
5 of 25 torsion outliers are listed below:

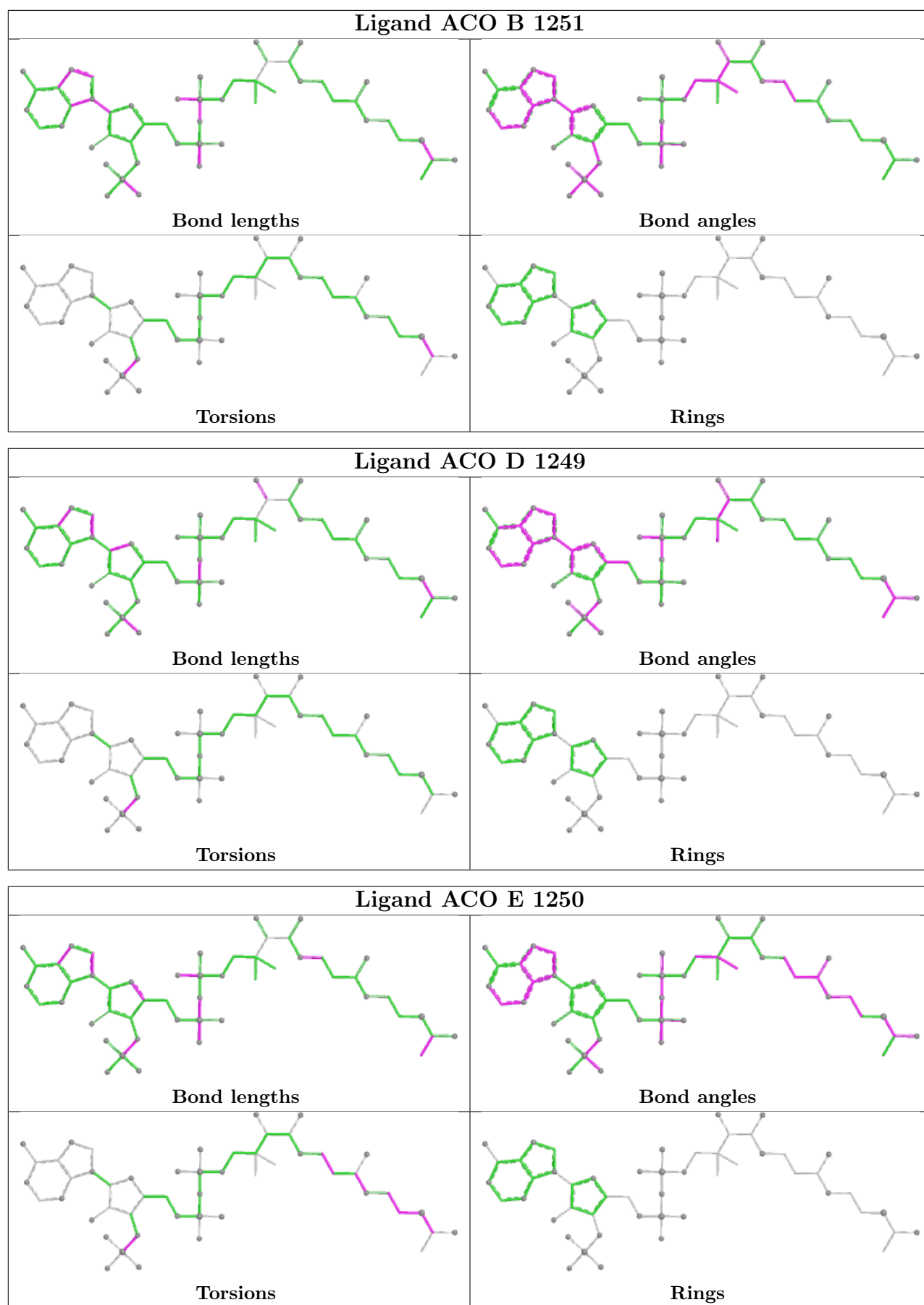
Mol	Chain	Res	Type	Atoms
4	E	1250	ACO	S1P-C2P-C3P-N4P
4	E	1250	ACO	C3P-C2P-S1P-C
4	F	1249	ACO	C5B-O5B-P1A-O2A
4	F	1249	ACO	CCP-O6A-P2A-O4A
4	F	1249	ACO	CDP-CBP-CCP-O6A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	239/276 (86%)	0.40	3 (1%) 75 73	22, 44, 56, 66	1 (0%)
1	B	248/276 (89%)	-0.18	3 (1%) 76 75	27, 33, 51, 64	3 (1%)
1	C	236/276 (85%)	0.62	9 (3%) 44 41	19, 45, 54, 60	1 (0%)
1	D	246/276 (89%)	-0.46	2 (0%) 82 81	15, 32, 45, 54	5 (2%)
2	E	241/276 (87%)	-0.37	3 (1%) 76 75	16, 33, 47, 60	2 (0%)
3	F	247/276 (89%)	-0.31	0 100 100	20, 35, 45, 55	2 (0%)
All	All	1457/1656 (87%)	-0.06	20 (1%) 73 72	15, 36, 52, 66	14 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	76	PHE	9.4
1	A	81	ALA	5.5
1	C	72	LEU	4.4
1	A	72	LEU	3.9
1	C	146	TRP	3.1

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

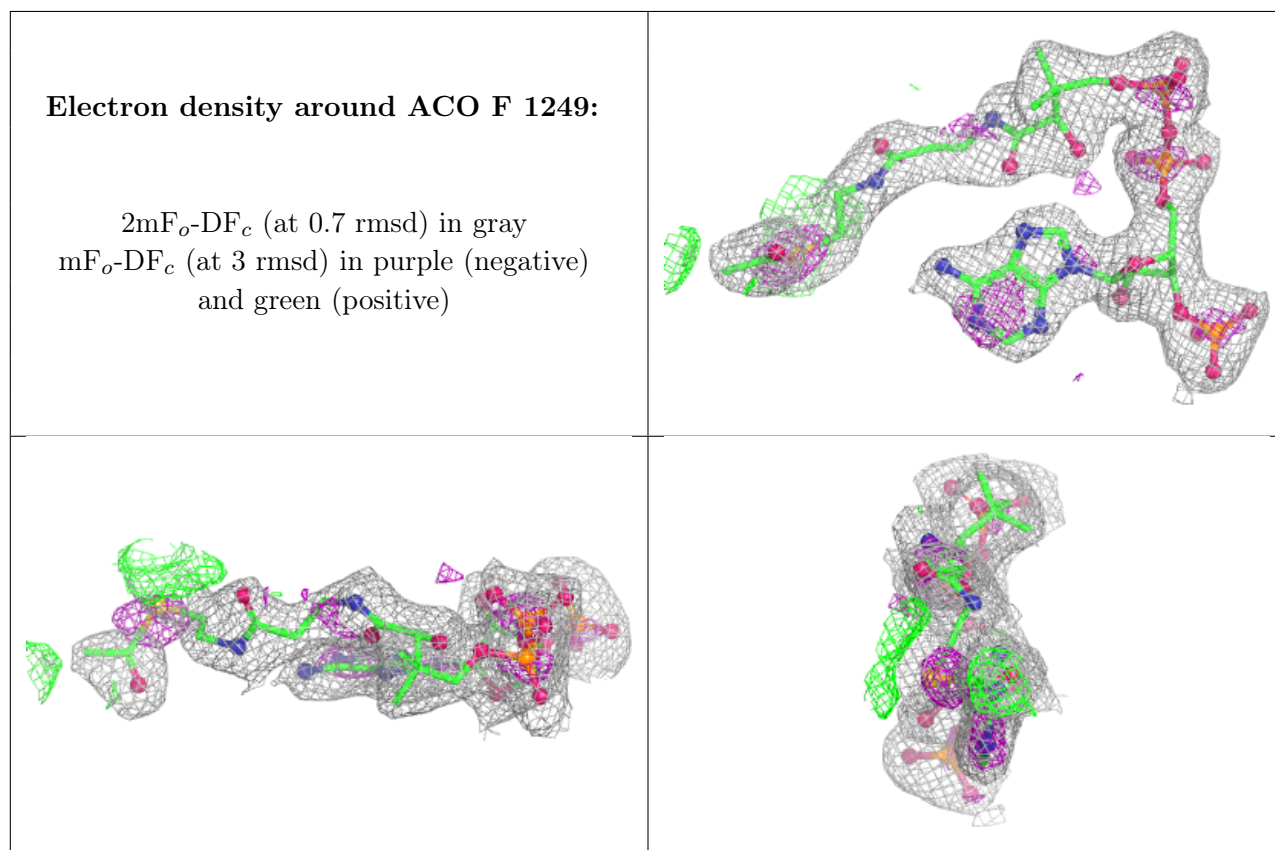
There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

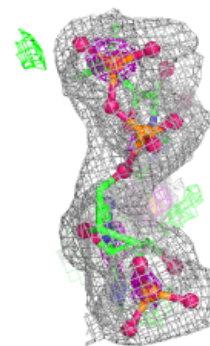
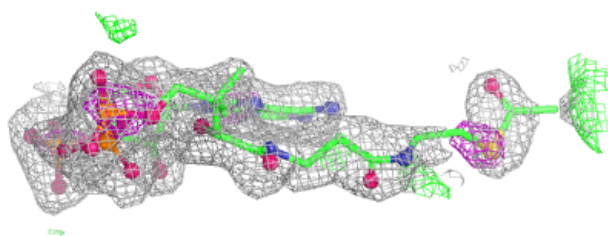
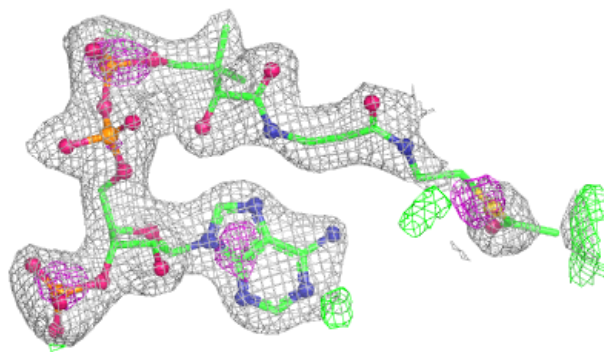
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACO	F	1249	51/51	0.90	0.10	38,44,52,66	0
4	ACO	E	1250	51/51	0.91	0.10	37,44,68,73	0
5	V55	D	1250	11/11	0.91	0.12	35,40,41,43	3
4	ACO	D	1249	51/51	0.93	0.09	32,40,52,62	0
4	ACO	B	1251	51/51	0.93	0.10	37,44,65,68	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

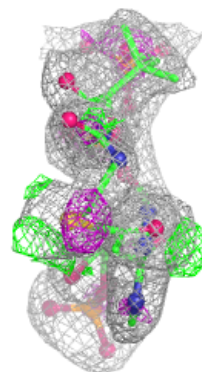
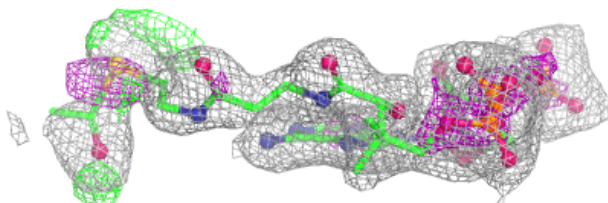
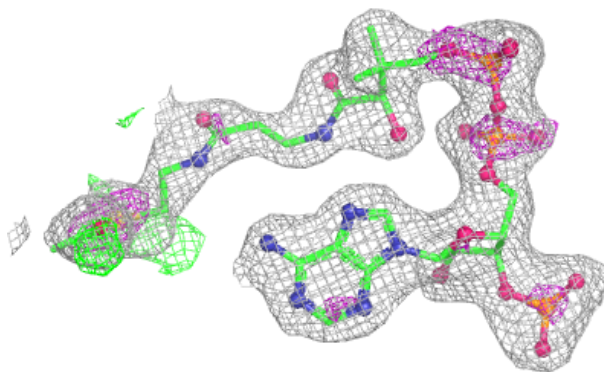


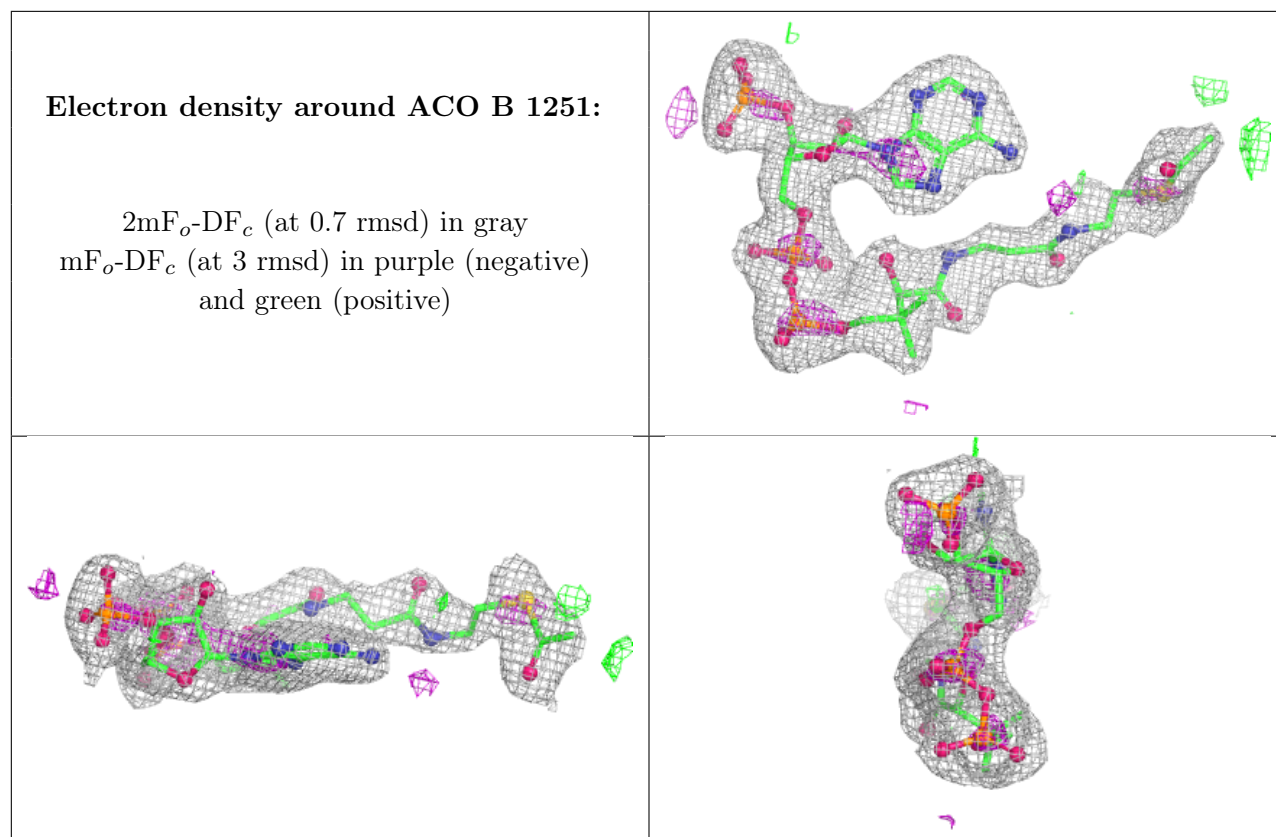
Electron density around ACO E 1250:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ACO D 1249:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





5.5 Other polymers [i](#)

There are no such residues in this entry.